201-16554S

IUCLID

Data Set

Existing Chemical	:	ID: 71888-89-6
CAS No.	:	71888-89-6
EINECS Name	:	Diisoheptyl phthalate
EC No.	:	276-158-1
Molecular Weight	:	362
Molecular Formula	:	C22H34O4

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Status	:	
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	05.07.2006
Revision date	:	
Date of last update	:	05.07.2006
Number of pages	:	32
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Contact person	:	Dr. Marian Stanley
Date	:	
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Town	:	22209 Arlington, VA
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Homepage	:	

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers: 68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6 and 111381-90-9 (see remark for names)

Remark : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers and names:

68515-50-4 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear (DHP)

71888-89-6 1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (DIHP)

27554-26-3 1,2,-benzenedicarboxylic acid, diisooctyl ester (DIOP)

68515-44-6 1,2-benzenedicarboxylic acid, diheptyl ester, branched and linear (DinHP)

111381-89-6 1,2-benzenedicarboxylic acid (C7, C9) ester, branched and linear (79P)

111381-90-9 1,2-benzenedicarboxylic acid, (C7,C11) ester, branched and linear (711P)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower molecular weight transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate subcategories. Of the phthalates in this subcategory, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

03.04.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	-45 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)
Remark	:	Manufacturer's data or handbook value
Test substance	:	diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability	:	(2) valid with restrictions Although the original reference was not retrieved and reviewed for quality, this robust summary has a reliability rating of 2 because the data are from a peer reviewed handbook that was developed for the purpose of identifying comprehensive and definitive physicochemical and biological data for numerous substances including phthalate esters.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (4)

Value	:	43 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)
Method	:	The calculated value was determined using MPBPWIN version 1.40, a subroutine within the computer program EPIWIN version 3.04. Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. The SMILES (Simplified Molecular Input Line Entry System) notation used to represent the structure of the substance in the model was: c1c(C(=O)OCCCCC(C)C)c(C(=O)OCCCCC(C)C)ccc1.
Remark	:	The EPIWIN suite of models is used by the US EPA for estimating chemicophysical properties of substances. However, the melting point calculation in EPIWIN provides erroneously high results for phthalate esters.
Test substance	:	diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability	:	(3) invalid The melting point calculation in EPIWIN provides erroneously high results for phthalate esters.

05.04.2006 (5)

2.2 BOILING POINT

Value	:	= 393.5 °C at 1013 hPa
Decomposition	:	no

Method	:	other: calculated value
Year	:	1999
GLP	:	
Test substance	:	other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)
Method	:	Boiling point calculated by MPBPWIN v1.41 subroutine in EPIWIN, which is based on the method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587. The SMILES (Simplified Molecular Input Line Entry System) notation used to represent the structure of the substance in the model was: c1c(C(=O)OCCCCC(C)C)c(C(=O)OCCCCC(C)C)ccc1.
Remark	:	The EPIWIN suite of models is used by the US EPA for estimating chemicophysical properties of substances.
Test substance	:	diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are not measured.
Flag	:	Critical study for SIDS endpoint

05.07.2006 (5)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.000000933 hPa at 25 °C
Decomposition	:	no
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for vapour pressure, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisoheptyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for diisoheptyl phthalate ester was 476.0 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
05.04.2006 (2)

Value : .0000108 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)

Method : Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04.
Vapor Pressure estimations performed by MPBPWIN are based on the average result of the calculation methods of Antoine and Grain. Both methods use boiling point for the calculation.
The SMILES (Simplified Molecular Input Line Entry System) notation used to represent the structure of the substance in the model was:
c1c(C(=O)OCCCCC(C)C)c(C(=O)OCCCCC(C)C)ccc1.
The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990.
A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Remark : The EPIWIN suite of models is used by the US EPA for estimating chemicophysical properties of substances.
Test substance : diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
05.04.2006 (5)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 6.87 at 25 °C
pH value :
Method : other (calculated)
Year : 2000
GLP :
Test substance : other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)

Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for partition coefficient, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisoheptyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for diisoheptyl phthalate ester was 476.0 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
05.07.2006 (2)

Partition coefficient : octanol-water
Log pow : 7.41 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance : other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)

Method : The value was calculated using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
The SMILES (Simplified Molecular Input Line Entry System) notation used to represent the structure of the substance in the model was:
c1c(C(=O)OCCCCC(C)C)c(C(=O)OCCCCC(C)C)ccc1.
Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Remark : The EPIWIN suite of models is used by the US EPA for estimating chemicophysical properties of substances.
Test substance : diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
05.04.2006 (5)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = .017 mg/l at 22 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :

pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Slow-Stir Water Solubility
Year	:	
GLP	:	no
Test substance	:	other TS: Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Result	:	The water solubility of diisoheptyl phthalate ester was determined as 0.017 mg/L, based on duplicate samples which each measured 0.017 mg/L. The water solubility of dihexyl phthalate, 0.07 mg/L was also determined in this study.
Test condition	:	Slow-stir water solubility vessels consisted of glass aspirator bottles with capacities ranging from 4 to 12 L. The spigots were fitted with short lengths of Tefzel tubing (approximately 10 cm 11 mm i.d.)and #13 glass stoppers. Bottles were solvent rinsed prior to use with a mixture of 1:1 methylene chloride:acetone followed by 2,2,4-trimethyl pentane. They were air dried in a laboratory fume hood and finally rinsed three times with the appropriate test water. A 4 cm glass-coated stir bar was placed in each bottle. The bottles were placed on magnetic stir plates and filled with the appropriate volume of water. Room temperature tests were performed at approximately 22 ° C. Test substance was added and stirred quiescently with little or no visible vortex until equilibrium was demonstrated. Quiescent mixing was stopped 1 h prior to sampling. Depending on the size of the vessel, a 100 -500 ml aliquot was removed from the respective vessels and some of this discarded sample was used to rinse the sample extraction bottles prior to sampling. This was intended to eliminate any sampling dead spots located in the vicinity of the sampling port. Sampling from the bottom sampling port also eliminated the possibility of contaminating the water samples with free product floating on the surface of the test bottles. Because all analyzed directly by automated static headspace GC-MS. The only sample preparation step was dilution into a 50 mg/l mercuric chloride solution. Duplicate samples were taken at each sampling interval. Phthalate ester SPE extraction was performed using an all glass extraction-filtering apparatus (HPLC mobile phase filter flask) fitted with a solvent conditioned Empore octadecyl (47 mm diameter) extraction disk. Sample volumes ranging from 500 to 3000 ml were extracted following the manufacturer 's referenced procedure. A 0.5 ml aliquot of o-terphenyl internal standard solution dissolved in ethyl acetate was added to the collection vial prior to eluting the extraction disk. The collected extracts were reduced to 0.5 ml final volumes under a gentle stream of nitrogen in a heating block. mixtures, these compounds were eluted with a relatively rapid temperature program to, as much as possible, elute the isomeric components as a single chromatographic peak. Samples were solvent extracted and analyzed by GC (gas chromatograph)-MSD (mass selective detector) using a Hewlett-Packard 5890 Series II GC equipped with a HP 5972 MSD, HP 7673A automatic injector, and a 30 m, 0.25 mm ID, 0.25 um df HP-5MS capillary column with 4 mm injection port liner. Three to five ul injections were made in the splitless mode with an injection port temperature of 275 C and MSD transfer line at 300 C.
Test substance	:	Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Reliability	:	(1) valid without restriction The study followed an accepted testing procedure for water immiscible, low solubility liquids. The study procedure and results were accepted in a peer reviewed journal. The data are consistent with known properties of similar high molecular weight phthalate ester substances.

Flag	:	Critical study for SIDS endpoint
05.04.2006		(11)
Solubility in	:	Water
Value	:	.00245 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Method	:	Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 7.41.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
05.04.2006		(5)
Solubility in	:	Water
Value	:	.02 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for water solubility, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisoheptyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for diisoheptyl phthalate ester was 476.0 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

05.04.2006 (2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	1 based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .00000000001774 cm³/(molecule*sec)
Degradation	:	= 50 % after 7.2 hour(s)
Deg. product	:	not measured
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)
Method	:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04. Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. The SMILES (Simplified Molecular Input Line Entry System) notation used to represent the structure of the substance in the model was: c1c(C(=O)OCCCCC(C)C)c(C(=O)OCCCCC(C)C)ccc1.
Remark	:	The atmospheric half-life value of 7.2 hours is equivalent to 0.6 days, based on the consideration that hydroxyl radicals needed for degradation are generated during the day light period (12 hours a day). The EPIWIN suite of models is used by the US EPA for estimating chemicophysical properties of substances.
Test substance	:	diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.07.2006 (5)

3.1.2 STABILITY IN WATER

Type	:	
t1/2 pH4	:	at °C
t1/2 pH7	:	3.4 year at 25 °C
t1/2 pH9	:	at °C
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: diisoheptyl phthalate ester (CAS No. 71888-89-6)
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67, a subroutine of the computer program EPIWIN version 3.04., that is based on work for EPA by T. Mill et al. The SMILES (Simplified Molecular Input Line Entry System) notation used to represent the structure of the substance in the model was: c1c(C(=O)OCCCCC(C)C)c(C(=O)OCCCCC(C)C)ccc1.
Remark	:	The EPIWIN suite of models is used by the US EPA for estimating

chemicophysical properties of substances.

Test substance : diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
12.05.2006 (5)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1997

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Select physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program [the SMILES (Simplified Molecular Input Line Entry System) notation used to represent the structure of the substance in the model was: c1c(C(=O)OCCCCC(C)C)c(C(=O)OCCCCC(C)C)ccc1]. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).
The input values used with the model were:
Molecular Weight: 363
Temperature: 25 °C
Log Kow: 6.87
Water Solubility: 0.017 mg/L
Vapor Pressure: 9.33E-7 hPa
Melting Point: -45°C

Result : Soil: 97.60%
Air: 0.14%
Water: <0.01%
Sediment: 2.17%
Suspended sediment: 0.07%
Biota: <0.01%

Test substance : diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are

calculated and not measured.

Flag : Critical study for SIDS endpoint
05.04.2006 (12)

Media : other: air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	363
Temperature	25° C
Log Kow	6.87
Water Solubility	0.017 g/m3
Vapor Pressure	.0000933 Pa
Melting Point	-45°C

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	14.4a
Water	120b
Soil	420c
Sediment	420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on read-across biodegradation data from 1,2-benzenedicarboxylic acid, di-C7 alkyl esters (CAS No. 71888-89-6): Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Result : Using the Mackay Level III calculation, the following distribution is predicted for 1,2,-benzenedicarboxcylic acid, diheptyl ester:

Compartment	% Distribution
Air	1.3
Water	9.1

	Soil	68.8
	Sediment	20.8
Test substance	:	diisoheptyl phthalate ester (CAS No. 71888-89-6)
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

12.05.2006 (12)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge, domestic, non-adapted
Concentration	:	50 mg/l related to Test substance related to
Contact time	:	28 day(s)
Degradation	:	= 82.2 (±) % after 28 day(s)
Result	:	
Deg. product	:	
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	1994
GLP	:	no
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, di-C7 alkyl esters (CAS No. 71888-89-6)

Result :

The biodegradation half-life <2 weeks. By day 28, 82.2% degradation of the test substance was observed. 10% biodegradation was achieved on approximately day 8, 50% biodegradation on approximately day 11, and >60% biodegradation on day 13.

By day 5, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted.

Test Substance:

Day	Percent Biodegradation (mean)
1	0
5	0.6
7	2.4
8	9.0
9	22.8
11	48.8
13	60.8
15	67.2
17	72.0
19	74.5
21	76.6
23	77.6
25	80.2
26	81.0
27	81.6
28	82.2

Positive Control:

Day	Percent Biodegradation (mean)
1	33.7
5	82.2
7	95.0

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test substance as calculated using results of an elemental analysis of the test substance.

Test condition : Activated sludge and test medium were combined prior to test substance addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test substance was tested in triplicate, controls and blanks were tested in duplicate.

Test substance (1,2-benzenedicarboxylic acid, di-C7 alkyl esters) concentration was approximately 50 mg/L. The positive control (sodium benzoate) concentration was approximately 50 mg/L. Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Test substance : 1,2-benzenedicarboxylic acid, di-C7 alkyl esters (CAS No. 71888-89-6)
No information on purity.

Conclusion : The test substance is readily biodegradable.

Reliability : (1) valid without restriction
This summary is rated a "1" and represents a key study because it followed an OECD standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

Flag : Critical study for SIDS endpoint
27.04.2006 (7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> .2
LL0	:	= .2
Limit test	:	yes
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1992
GLP	:	yes
Test substance	:	other TS: diisoheptyl phthalate (CAS No. 71888-89-6)

Method : This study was designed as a limit test with one exposure solution. The treatment solution, 100 mg/L, was prepared by adding sufficient test substance via syringe to 19.5 L of laboratory blend water in a sealed 20L glass carboy. The stock solution was mixed for 24 hours with a vortex of <10%. Mixing was performed using a magnetic stir plate and teflon stir bar. After mixing, the solution was allowed to settle for approximately one hour and the Water Accommodated Fraction (WAF) was then siphoned from the bottom of the mixing vessel and added to the test vessel. The siphon was placed in the carboy prior to test material addition.

Test vessels were 4.0 L aspirator bottles containing approximately 4.5 L of solution, sealed with no headspace. Three replicates of the treatment and control were tested, each containing 5 fish. Approximately 80% of the treatment solution was renewed daily from a freshly prepared WAF.

Exposure solutions were control and 100 (nominal) mg/L, which measured 0.0 and 0.2 mg/L, respectively, in new solutions on day 1.

Mean test temperature was 15 Deg C. Light intensity ranged from 568 to 570 Lux with 16 hr light and 8 hr dark intervals. Dissolved oxygen was 8.8 to 9.5 mg/L in control and "new" treatment solutions and 6.4 to 7.7 mg/L in control and "old" treatment solutions. The pH ranged from 7.0 to 8.4 in control and "new" treatment solutions and 7.0 to 7.5 in control and "old" treatment solutions.

Treatment Level (mg/L)	Dissolved Oxygen (mg/L)	pH	Temperature (Deg. C)
Control	6.8 - 9.5	7.0 - 8.3	15.0 - 16.0
100	6.4 - 9.5	7.1 - 8.4	15.0 - 16.0

Fish supplied by Thomas Fish Co.: age = approximately 4 weeks; mean wt. = 0.162 g; mean total length = 2.9 cm; test loading = 0.18 g fish/L.

Result : 96-hour LL0 = 100 mg/L and LL50 > 100 mg/L based upon nominal values
96-hour LL0 = 0.2 mg/L and LL50 > 0.2 mg/L based upon measured values

No test related mortality at the reported test substance loading (a saturated exposure solution prepared at a loading of 100 mg/L)..

The fish were slightly smaller than the guideline suggestion of 4.0 to 6.0cm, which were purposely selected to help maintain oxygen levels in the closed system.

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID). Analytical measurements were taken to confirm test material presence in test solutions and absence in control.

Nominal Loading (mg/L)	Fish Total Mortality (@ 24, 48, 72, 96 hrs)*
Control	0, 0, 0, 0
100	0, 1**, 0, 0

*15 fish added to each control and treatment level at test initiation
** Mortality was not test related

Total motality was1 fish. However, it is not believed to be test related. During observations on day 0, one fish in the 100 mg/L treatment was observed as missing an eye. This conditions is believed to have existed prior to the start of the test and was overlooked during the randomization procedure. This fish subsequently died on day 2 of the study and is considered to be non-test related. It was not included in the evaluation of the study data.

Test substance : Diisoheptyl phthalate (CAS No. 71888-89-6)
Purity: unstated, but believed to be 100% active ingredient.

Conclusion : Diisoheptyl phthalate is not acutely toxic to rainbow trout (Oncorhynchus mykiss) based on the data from this study. These toxicity data are consistent with valid data for several high molecular weight phthalate esters as summarized by Brown et al. (1998), Staples et al. (1997), and Rhodes et al. (1995). These data show that high molecular weight phthalate esters, including diisoheptyl phthalate ester, do not produce acute toxicity to rainbow trout.

The study design was selected because the water solubility of the test substance is low (significantly less than 100 mg/L). The test substance is a not pure, but rather complex. The alkyl group is primarily a C7, but can include some C6 and C8. Additionally, the alkyl groups contain several different isomers for each carbon number.

Reliability : (1) valid without restriction
This study is rated a "1" because it followed an accepted test guideline, used appropriate testing procedures, and applied GLP. Additionally, the data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.

Flag : Critical study for SIDS endpoint
27.04.2006 (1) (8) (15) (16)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species : Oncorhynchus mykiss (Fish, fresh water)
Endpoint : other: survival, growth, and sex ratio
Exposure period : 271 day(s)

Unit	:	
Analytical monitoring	:	yes
Method	:	other: OECD Guide-line 215, Fish juvenile growth test
Year	:	2000
GLP	:	yes
Test substance	:	other TS: diisoheptyl phthalate (CAS No. 71888-89-6)
Method	:	Using the OECD Guide-line 215, Fish juvenile growth test, a single dietary concentration of 1000 ug test substance/g feed (Fin Fish Starter, No.1 and 2, Zeigler Bros. Inc.) was investigated to determine if effects could be detected under high, continuous dietary exposure in comparison with a control group fed an uncontaminated diet. Exposure was initiated immediately after yolk-sac resorption (fish were approximately 4 weeks old) and continued for 271 days. Chronic endpoints investigated during the study included survival, growth, and sex ratio as determined by histological examination of the gonads.
Remark	:	The objective of this study was to extend the available effects database to a C7 phthalate [di-isoheptyl phthalate (DIHP)] by determining if prolonged dietary exposure to this compound could produce chronic effects in rainbow trout. Past aquatic toxicology studies have shown that di-alkyl phthalates with alkyl chain lengths of greater than six carbons do not pose a chronic toxicity hazard to aquatic organisms when exposed to these substances via the water. These findings are consistent with the low water solubility and bioconcentration potential of these substances. However, the diet provides another potential and likely route of chronic exposure that warranted consideration.
Result	:	NOEC = 1 mg test substance/g feed DIHP in the diet was confirmed analytically throughout the test and found to be in good agreement with the nominal level, which was 1000 ug/g feed. No DIHP-related effects were observed through the 271-day exposure. At the end of the dietary exposure period, DIHP and MIHP were present in the gut at concentrations of 301 and 122 nmole, representing 25% and 10%, respectively, of the daily dose. However, neither DIHP nor MIHP were detected in fish muscle above background levels of 0.104 and 0.018 µg/g, respectively, as measured in the control fish.However, MIHP was detected at very low levels in the liver confirming internal exposure of this metabolite arising from dietary exposure to DIHP. In the depuration phase of this study, MIHP was completely eliminated from the liver of exposed fish in 2 days.
Test substance	:	Diisoheptyl phthalate (CAS No. 71888-89-6) Purity: unstated, but believed to be 100% active ingredient.
Conclusion	:	NOEC = 1 mg test substance/g feed The lack of chronic effects observed in this study is consistent with other recent dietary toxicity studies with fish on C8-C10 phthalates.
Reliability	:	(1) valid without restriction This summary has a reliability rating of 1 because it followed a guideline study. However, the report is in draft and currently only an abstract is available for review.
Flag	:	Critical study for SIDS endpoint

27.04.2006 (3)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia magna (Crustacea)
Endpoint	:	reproduction rate
Exposure period	:	21 day(s)
Unit	:	mg/l
NOEC	:	= .92 measured/nominal
EC50	:	> .92 measured/nominal

Analytical monitoring : yes
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year : 1984
GLP : yes
Test substance : other TS: Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Method : The test method followed the Daphnid chronic testing procedure described in OECD guideline 202 (1984) with the use of a dispersant, castor oil 40-ethoxylate (Marlowet 40), in accordance with guideline specifications.
Result : Daphnia parent (Po) survival, reproduction (cumulative number of offspring, F1, per live parent), and parent length were evaluated as the biological endpoints. Diisoheptyl phthalate ester showed no effect on survival, reproduction, and length at a loading of 1.0 mg/L test substance and 10 mg/L dispersant under the conditions of this test.

	Po % Mortality	Mean F1/ Surviving Po	Po Mean Length
Test Substance	10	110 (sd=12)	4.2 (sd=0.14)
Control	0	93 (sd=9)	4.1 (sd=0.17)

Test condition : Test substance exposure solutions were prepared using stock dispersions prepared by adding 100 mg substance and 1000 mg dispersant (castor oil 40-ethoxylate; Marlowet 40), then bringing the test solution to 1 L by adding dilution medium. The dilution medium was Elendt's medium (Elendt and Bias, 1990), which was pH adjusted to 8 and aerated for >2 hours prior to use.

Ten replicate test systems with 1 daphnid each (< 24 hours old) were prepared in glass beakers with loose fitting lids. Each beaker contained 80 ml of exposure solution with a depth of approximately 5 cm. The photoperiod was controlled to 16 hours light and 8 hours dark with a 15 minute transition period.

The exposure solution was renewed every Monday, Wednesday, and Friday. On each renewal day the parent organism (Po) was transferred to a new exposure solution and neonates (F1) were counted. Water quality measurements including dissolved oxygen concentration and pH were determined at every renewal for the new and old exposure and control solutions. Test conditions were:

Temperature = 20 +/- 1.0 degree C
Water harness = >140 mg/L (as CaCO3)
Alkalinity = >100 mg/L (as CaCO3)
pH = approximately 8
Dissolved oxygen = 8-9 mg/L

Standard daily feeding rates with the cultured alga, Chlorella vulgaris, was supplemented with microencapsulated food, "Frippak Booster".

Test substance analyses of new and old exposure solutions were performed using gas chromatography with flame ionization detection, after a hexane extraction. The mean measured test substance concentrations were 1.0 mg/L in new exposure solutions and 0.85 mg/L in old exposure solutions, which represents 100 and 85%, respectively, of the nominally added test substance.

Test substance : Diisoheptyl Phthalate Ester (CAS No. 71888-89-6); purity >99.5%
Conclusion : Chronic invertebrate (Daphnia magna) toxicity data reported for diisoheptyl phthalate ester are consistent with valid data for several high molecular weight phthalate esters as summarized by Brown et al. (1998), Staples et al. (1997), and Rhodes et al. (1995). These data show that high molecular weight phthalate esters, including diisoheptyl phthalate ester, do not produce chronic toxicity to Daphnia magna. Testing was conducted at a loading that exceeds the water solubility of diisoheptyl phthalate ester (0.017 mg/L; Letinski et al., 2002) after it was demonstrated that such a

procedure was able to satisfactorily disperse the test substance and that it prevented floatation of the test organism, a documented problem that can occur when evaluating the toxicity of similar substances.

Reliability : (1) valid without restriction
This study is rated a "1" because it followed an accepted test guideline, used appropriate testing procedures, and applied GLP. The study procedure and results were accepted in a peer reviewed journal. Additionally, the data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.

Flag : Critical study for SIDS endpoint
05.04.2006 (1)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 10000 mg/kg bw
Species	:	rat
Strain	:	Wistar
Sex	:	male
Number of animals	:	35
Vehicle	:	no data
Doses	:	
Method	:	other
Year	:	1978
GLP	:	no data
Test substance	:	other TS: Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Remark	:	There were no deaths at any dose level or time point. Signs of toxicity included diarrhea, lethargy and piloerection. At all dose levels, these signs were observed in the early stages of the test. Most of these signs were diminished during the later part of the observation period.
Test condition	:	Seven groups (5 per group) of male Wistar rats at least 8 weeks of age were dosed with diisoheptyl phthalate by syringe at doses of 1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg. The rats were observed at 1, 2, 4 and 6 hours after dosing and once daily for 14 days. Mortality, toxicity and pharmacological effects were recorded. On day 14, the survivors were sacrificed. All animals were examined for gross pathology
Test substance	:	1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)
Conclusion	:	The test material was not acutely toxic at levels up to 10.0 g/kg.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

27.04.2006 (14)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	= 3160 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	2
Vehicle	:	
Doses	:	
Method	:	other (calculated)
Year	:	1979
GLP	:	no
Test substance	:	other TS: Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Remark	:	There were no deaths at the tested dose level. Slight erythema was noted at the 24 hour observation only. At necropsy, all animals were observed with dilated hearts.

Test condition	:	A single dose level of 3160 mg/kg body weight was used. On the day prior to dosing the fur of each rabbit was clipped from the abdomen. The skin also was abraded. The test material was applied directly to the skin and the area was wrapped with gauze and an impervious plastic sleeve. The wraps were removed after 24 hours and dermal observations recorded. General observations were recorded immediately after dosing, 2 and 4 hours; and once daily thereafter for 14 days. Observations for skin irritation were recorded 30 minutes after removal of the wrap and at Days 3, 7, 10, and 14. Body weights were recorded prior to dosing and at 14 days. Gross necropsies were conducted on all animals that were sacrificed at the termination of the study.
Test substance	:	1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)
Conclusion	:	The test material was not acutely toxic at levels up to 3.16 g/kg.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

27.04.2006 (13)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Bacterial
Test concentration	:	250, 500, 1000, 2500, and 5000 mg/ml
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1995
GLP	:	yes
Test substance	:	other TS: Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Method	:	Statistical Methods: The mean revertant colony count and standard deviation were determined for each dose point (Snedecor and Cochran, 1989). An individual dose was considered positive if the mean revertant count on the test plates was equal to or greater than three times the mean number of spontaneous revertants on the vehicle control plates.
Result	:	In both the initial and repeat assays the test substance beaded on the plate at concentrations of 500 mg/plate and greater. However, the test substance was soluble in the vehicle, DMSO. The test material did not induce a significant difference in revertant colonies in tester strains TA98, TA100, TA1535, TA1537 or TA1538 at any dose level with or without metabolic activation in either the initial or repeat assays.

Test condition	:	Prior to assay initiation, a toxicity pretest was performed using tester strain TA98. Based on these results, the doses for the final assay were determined. In the definitive assay, each of the four strains was dosed either with the test substance; a vehicle control (DMSO); or a nontreated control and a positive control. Positive controls were as follows: 2-aminoanthracene (all strains with S9); 2-nitrofluorene (TA98, TA1538 without S9); N-methyl-n-nitro-n-nitrosoguanidine (TA100, TA1535 without S9) and 9-aminoacridine (TA1537 without S9). There were 3 plates/dose group/strain/treatment. The test results were verified by repeating the assay. Both the initial and repeat assays were terminated approximately 48 hours following dose initiation.
Test substance	:	1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)
Conclusion	:	Under conditions of this study, diisoheptyl phthalate was inactive in the Ames mutation assay.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

05.07.2006 (6)

Type	:	Chromosomal aberration test
System of testing	:	Non-Bacterial
Test concentration	:	499, 1250, 2500, 3750, and 4990 mg/ml
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473
Year	:	1991
GLP	:	yes
Test substance	:	other TS: Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Method	:	Statistical Methods: A statistically significant ($P < 0.05$) difference for one dose point and a significant trend ($P < 0.015$) were considered evidence of a positive response; significant differences for two or more doses indicated the trial was positive.
Result	:	In the 10 hour harvest assay, no significant increase in cells with chromosomal aberrations was observed at the doses analyzed. Similarly, no significant increase in cells with chromosomal aberrations was observed in the 20 hour assay. Evidence that the metabolic system was working properly was demonstrated by the cyclophosphamide-induced increased incidence in aberrations.
Test condition	:	Results from a rangefinding assay were used to determine the dose range used in the study. In the rangefinding assay, the cultures were incubated for 25-26 hours with 5-bromo-2'deoxyuridine. In the chromosomal aberration assay, replicate cultures were used at each dose level. Single cultures were used for the negative controls, solvent control, and at each of two doses of the positive control. Solvent controls were cultures containing the solvent for the test material. The positive controls used in this assay were: mitomycin C (without S9) and cyclophosphamide (with S9). In the assay without S9, a harvest time of 20 hours was used. In the assay with S9, harvest times of 10 and 20 hours were used.
Test substance	:	1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)
Conclusion	:	No induction of chromosomal aberrations was observed in CHO cells in the presence or absence of S9.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

05.07.2006 (10)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Gestation days 6-15
Frequency of treatm.	:	Daily
Duration of test	:	9 days
Doses	:	0, 100, 300, or 750 mg/kg/day
Control group	:	yes
NOAEL maternal tox.	:	= 750 mg/kg bw
NOAEL teratogen.	:	= - 300 mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	1997
GLP	:	yes
Test substance	:	other TS: Diisoheptyl Phthalate Ester (CAS No. 71888-89-6)
Method	:	ANOVA; Dunnett's Test; Dunn's Summed Rank Test.
Result	:	Maternal Effects: There were dose-related increases in mean absolute and relative maternal liver weights that were statistically significant in the 300 and 750 mg/kg dams compared with controls. These increases were consistent with the known ability of certain other alkyl esters of 1,2-benzenedicarboxylic acid to cause peroxisome proliferation and were considered to be a physiological adaptation. Thus, under the condition of this study, no clear maternal toxicity was identified. Embry/fetal Effects: At doses of 300 mg/kg or less, there were no treatment-related or biologically important fetal malformations, embryolethality, or fetal weight reduction. Evidence of growth retardation and increased embryo/fetal death was observed in the high dose (750 mg/kg) group compared with controls. Additionally, there was an increased incidence of external, visceral and skeletal malformations/variations in the 750 mg/kg compared with control. External, visceral and skeletal malformations/variations which were statistically significant as compared to controls on a per fetus and per litter basis are listed to provide detail. External: anasarca, red amniotic fluid, exencephaly, cranioschisis, apparent anophthalmia, apparent micophthalmia, cleft palate, atresia tail, and malformed tail Visceral: abnormal origin of the subclavia artery, agenesis of the innominate artery, ectopic testes/ovaries Skeletal: fused/malformed sternebrae, fused ribs, thoracic centra/arch agenesis and fused/short rib anlage.
Test condition	:	The test material was administered by oral gavage to 25 confirmed-mated female rats at doses of 0 (corn oil only), 100, 300, and 750 mg/kg at a dose volume of 5 ml/kg once daily from gestation day (GD) 6 through GD 20. Clinical observations were made daily during gestation. Body weight and food consumption measurements were made on GD 0, 6, 9, 12, 15, 18, and 21. On GD 21, animals were sacrificed and cesarean sections were performed. Gross necropsies were performed, liver weights and uterine

weights with ovaries attached were recorded, uterine contents were examined, and the required uterine implantation data were recorded. All live fetuses were weighed, sexed externally, and examined externally for gross malformations.

Test substance : 1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (diisoheptyl phthalate)

Conclusion : Under the conditions of this study the test material was considered embryolethal, fetotoxic, and a selective developmental toxicant at a dose of 750 mg/kg.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

27.04.2006 (9)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

05.07.2006

10.3 RISK ASSESSMENT